Linoleic acid ethyl ester

Other names:	(Z,Z)-9,12-octadecadienoic acid, ethyl ester
	9,12-Octadecadienoic acid (Z,Z)-, ethyl ester
	Ethyl cis,cis-9,12-octadecadienoate
	Ethyl linolate
	Mandenol
	ethyl (Z,Z)-9,12-octadecadienoate
	ethyl (Z,Z)-9,12-octadecadienoate
	ethyl linoleate
	linoleic acid, ethyl ester
Inchi:	InChI=1S/C20H36O2/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20(21)22-4-2/h8-9,
InchiKey:	FMMOOAYVCKXGMF-MURFETPASA-N
Formula:	C20H36O2
SMILES:	CCCCCC=CCC=CCCCCCCCC(=O)OCC
Mol. weight [g/mol]:	308.50
CAS:	544-35-4

Physical Properties

Property code	Value	Unit	Source
gf	44.04	kJ/mol	Joback Method
hf	-466.49	kJ/mol	Joback Method
hfus	50.75	kJ/mol	Joback Method
hvap	69.19	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.363		Crippen Method
mcvol	291.500	ml/mol	McGowan Method
pc	1120.05	kPa	Joback Method
rinpol	2162.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2171.00		NIST Webbook
rinpol	2166.00		NIST Webbook
rinpol	2162.00		NIST Webbook
rinpol	2169.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2156.00		NIST Webbook
rinpol	2177.00		NIST Webbook
rinpol	2144.00		NIST Webbook

rinpol	2164.00	NIST Webbook
rinpol	2152.00	NIST Webbook
rinpol	2159.00	NIST Webbook
rinpol	2155.00	NIST Webbook
rinpol	2140.00	NIST Webbook
rinpol	2193.00	NIST Webbook
rinpol	2162.90	NIST Webbook
rinpol	2139.00	NIST Webbook
rinpol	2139.00	NIST Webbook
rinpol	2141.00	NIST Webbook
rinpol	2151.00	NIST Webbook
rinpol	2145.00	NIST Webbook
rinpol	2162.00	NIST Webbook
rinpol	2162.00	NIST Webbook
rinpol	2162.00	NIST Webbook
rinpol	2141.00	NIST Webbook
rinpol	2155.00	NIST Webbook
rinpol	2159.00	NIST Webbook
rinpol	2177.00	NIST Webbook
rinpol	2159.00	NIST Webbook
rinpol	2165.00	NIST Webbook
ripol	2510.00	NIST Webbook
ripol	2486.00	NIST Webbook
ripol	2511.00	NIST Webbook
ripol	2538.00	NIST Webbook
ripol	2530.00	NIST Webbook
ripol	2515.00	NIST Webbook
ripol	2534.00	NIST Webbook
ripol	2536.00	NIST Webbook
ripol	2505.00	NIST Webbook
ripol	2521.00	NIST Webbook
ripol	2520.00	NIST Webbook
ripol	2519.00	NIST Webbook
ripol	2528.00	NIST Webbook
ripol	2532.00	NIST Webbook
ripol	2553.00	NIST Webbook
ripol	2530.00	NIST Webbook
ripol	2530.00	NIST Webbook
ripol	2491.00	NIST Webbook
ripol	2488.00	NIST Webbook
ripol	2491.00	NIST Webbook
ripol	2514.00	NIST Webbook
ripol	2510.00	NIST Webbook
ripol	2553.00	NIST Webbook

ripol	2524.00		NIST Webbook
tb	741.61	K	Joback Method
tc	919.70	K	Joback Method
tf	377.16	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.13	J/mol×K	741.61	Joback Method
cpg	961.38	J/mol×K	919.70	Joback Method
cpg	946.80	J/mol×K	890.02	Joback Method
cpg	931.49	J/mol×K	860.34	Joback Method
cpg	915.41	J/mol×K	830.65	Joback Method
cpg	898.51	J/mol×K	800.97	Joback Method
cpg	880.77	J/mol×K	771.29	Joback Method
dvisc	0.0026411	Pa×s	328.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0024287	Pa×s	333.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0022414	Pa×s	338.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0020753	Pa×s	343.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0019270	Pa×s	348.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0017727	Pa×s	353.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0016757	Pa×s	358.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0015685	Pa×s	363.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0081875	Pa×s	278.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0070842	Pa×s	283.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0061652	Pa×s	288.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0054231	Pa×s	293.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0048073	Pa×s	298.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel
dvisc	0.0043074	Pa×s	303.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel

dvisc	0.0038539	Pa×s	308.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0034060	Pa×s	313.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0031608	Pa×s	318.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
dvisc	0.0028291	Pa×s	323.15	Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel	
hvapt	72.60	kJ/mol	472.50	NIST Webbook	
pvap	9.33	kPa	537.69	Vapor liquid equilibrium of fatty acid ethyl esters determined using DSC	
pvap	9.33	kPa	537.39	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry	
pvap	8.00	kPa	527.47	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry	
pvap	6.67	kPa	520.91	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry	

pvap	5.33	kPa	515.70	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	4.00	kPa	510.65	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	2.67	kPa	501.94	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry
pvap	1.33	kPa	486.64	Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination of the vapor pressure of ethyl esters by Differential Scanning Calorimetry:	https://www.doi.org/10.1016/j.jct.2011.01.017
Vapor-liquid equilibrium of fatty acid ethyl esters determined using DSC:	https://www.doi.org/10.1016/j.tca.2010.10.002
Densities and Viscosities of Minority Fatty Acid Methyl and Ethyl Esters Present in Biodiesel:	https://www.doi.org/10.1021/je1012235

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume